Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

1. (Original) A method for determining properties of products from a combinatorial chemical library P using features of their respective building blocks, the method comprising the steps of:

(1) determining at least one feature for each building block in the combinatorial library P, $\{a_{ijk},\ i = 1,2,\ldots,r;\ j = 1,2,\ldots,r_i;\ k = 1,2,\ \ldots,\ n_i\}$, wherein r represents the number of variation sites in the combinatorial library, r_i represents the number of building blocks at the i-th variation site, and n_i represents the number of features used to characterize each building block at the i-th variation site;

(2) selecting a training subset of products $\{\boldsymbol{p}_i,\ i = 1,2,\ldots,\ m;\ \boldsymbol{p}_i \in P\}$ from the combinatorial library P;

(3) determining q properties for each compound $\boldsymbol{p}_i$ in the selected training subset of products, wherein $\boldsymbol{y}_i$ $\{y_{ij},\ i = 1,2,\ldots,m, j = 1,2,\ldots,q\}$ represents the determined properties of compound $\boldsymbol{p}_i$, and wherein q is greater or equal to one;

(4) identifying, for each product $\boldsymbol{p}_i$ of the training subset of products, the corresponding building blocks $\{t_{ij},\ t_{ij} = 1,2,\ldots,\ r_j, j = 1,2,\ \ldots,\ r\}$ and concatenating their features determined in step (1) into a single vector $\{\boldsymbol{x}_i = \boldsymbol{a}_{1t_{i1}} \mid \boldsymbol{a}_{2t_{i2}} \mid \boldsymbol{a}_{rt_{ir}}\}$;

(5) using a supervised machine learning approach to infer a mapping function f that transforms input values $\boldsymbol{x}_i$, to

output values y_i, from the input/output pairs in the training set $T = \{(x_i, y_i),\ i = 1, 2, \ldots, m\}$;

(6) identifying, after the mapping function f is determined, for a product $p_z \in P$, the corresponding building blocks $\{t_{zj},\ j = 1, 2, \ldots, r\}$ and concatenating their features, $a_{1t_{z1}}, a_{2t_{21}}, \ldots, a_{rt_{zr}}$, into a single vector $\{x_z = a_{1t_1} | a_{2t_2} | \ldots | a_{rt_r}\}$, and

(7) mapping $x_z \rightarrow y_z$, using the mapping function f determined in step (5), wherein y_z represents the properties of product p_z.

2. (Original) The method of claim 1, wherein step (1) comprises the step of:

using a measured value as a feature for each building block.

3. (Original) The method of claim 1, wherein step (1) comprises the step of:

using a computed value as a feature for each building block.

4. (Original) The method of claim 1, wherein step (3) comprises the step of:

using a measured value as a property for each product of the training subset.

5. (Original) The method of claim 1, wherein step (3) comprises the step of:

using a computed value as a property for each product of the training subset.

6. (Original) The method of claim 1, wherein step (5) comprises the step of:

training a multilayer perceptron.

7. (Original) The method of claim 1, wherein

at least one of the features determined in step (1) is the same as at least one of the properties determined in step (3).

8. (Original) The method of claim 1, wherein

the building blocks comprise a plurality of reagents used to construct the combinatorial library *P*.

9. (Original) The method of claim 1, wherein

the building blocks comprise a plurality of fragments of a plurality of reagents used to construct the combinatorial library *P*.

10. (Original) The method of claim 1, wherein

the building blocks comprise a plurality of modified fragments of a plurality of reagents used to construct the combinatorial library *P*.

11. (Original) The method of claim 1, wherein step (2) comprises the step of:

selecting a training subset of products at random.

12. (Original) The method of claim 1, wherein step (2) comprises the step of:

selecting a training subset of products using a combinatorial design method to cover all pairwise combinations of building blocks.

13. (Original) The method of claim 1, wherein step (2) comprises the step of:

selecting a training subset of products using a diversity metric to select a diverse subset of products.

Claims 14 to 40 (Cancelled).